

Molecular Thermodynamics of Nanoparticle-Polymer Systems

Monte-Carlo Computer Simulation of Chemical Potentials – Meredith

Nanoscale colloidal particles, as well as inorganic phases synthesized in situ in organic materials, display fascinating electronic, optical, thermal, and reinforcement properties as a consequence of their dimensions. Stable dispersions of nanoscale colloids may find applications in drug delivery, medical diagnostics, nanopatterning and nanocomposites. The self-assembly of nanoparticles into ordered crystalline arrays offers an attractive route to fabrication of a new generation of optical and electronic devices.

Unfortunately, robust molecular based models of these complex multiscale mixtures are still in their

infancy and relationships between molecular parameters and nanoparticle phase behavior are determined often by trial-and-error experimentation. A major contribution to this complexity is the adsorption of surface modifiers and the subsequent change in their available conformations.

Towards this goal, we recently developed a novel application of the expanded ensemble Monte Carlo (EEMC) simulation method that allows accurate calculation of the chemical potentials of organically-modified nanoparticles. Knowledge of the modifier chain length, concentration and particle size dependence of chemical potential can be used to predict conditions under which nanocolloids disperse, flocculate, or self-assemble. We are using the simulation technique to understand the structure and free energy of polymers around nanoparticles (Figure 1) and to probe the interparticle forces between nanoparticles immersed in polymer solutions (Figure 2).

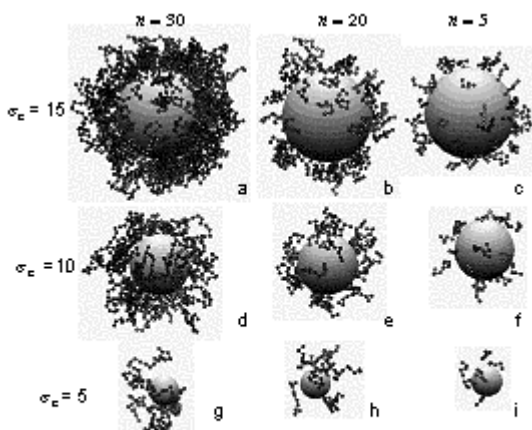
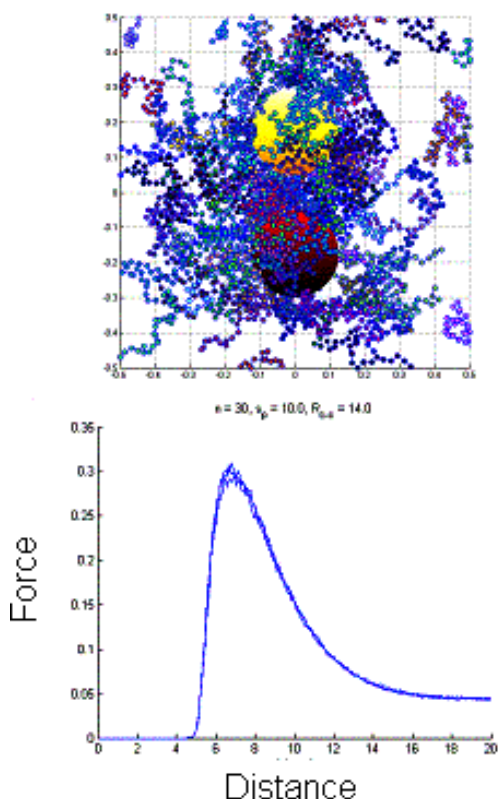


Figure 1. Snapshots of the equilibrated configurations for different particle sizes (n) and polymer chain lengths (σ_c).

Figure 2



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